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Study the Dynamic Behaviour of Distillation Column with Fundamental Modelling and Simulation by MATLAB

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Abstract— **Distillation columns are very substantial unit operations in process industries. In the present work, we reviews some techniques of modelling and simulation of distillation columns and explain with the help of MATLAB model for binary continuous distillation column. Simulation studies are often used to examine the operational behaviour of distillation column. A rigorous model for the simulation of the steady state behaviour of the distillation column. MESH equation, which actually represent the behaviour of the distillation column has been solved through MATLAB, in order to study the effect of different parameter. With the MATLAB software we study the dynamic behaviour of the product composition with the feed change with the time. In this paper the effect of the feed condition and the feed composition on the steady state behaviour. Developed code has been used to study the column and the result show that the composition response to disturbance are close to the response of first order system and also the response to change in feed composition has larger gain than the response to change in feed flow rate. Validation of the developed code has been using by the other author and is to be found in good agreement.**

Keywords- Binary Distillation Column, Relative Volatility, Modeling and Simulation, MATLAB

I. INTRODUCTION

Distillation column are most studied unit operation in chemical industries. Distillation is a process of separating mixtures based on differences in their volatilities in a boiling liquid mixture. Distillation process may be classified in two categories namely binary distillation and multicomponent distillation. It is used to separate a mixture into its components by the application and removal of heat. It consumes a huge amount of energy in both heating and cooling operations. There are many types of distillation columns based on different classifications such as: batch, conduct, tray, packed. In this paper we focus on continuous binary distillation columns since continuous columns are mostly used in industry. The objective of analysis mathematical model is to develop for binary distillation column. The model is constructed based on the physical properties of the system, such as the preservation of mass, energy and momentum. The mathematical models range from simple to rigorous models depending on the levels of complexity and the assumptions

A continuous distillation column shown in Fig. 1. The column has N stages on which the vapor liquid equilibriums occur. The feed enters the column on the stage N_F. This stage divides the column into a rectifying section and a stripping section. Near the bottom of the column is a reboiler which provides energy to the column. The mixture is heated to form a flow of vapor rising up inside the column. In the stripping section, the less volatile component is enriched while in the rectifying section the more volatile component is enriched. The top product is condensed by the condenser from which there is a reflux flow back to the top of the column to enhance the purity of the product.

In distillation column our main problem is to control it because of their highly nonlinear characteristics. It is defined as in distillation column in their multiple input and multiple output so there is several disturbance .We can easily understand the non-linearity of distillation column. We can get if the product is purer the system become more non-linear [3]. The term rectification is derived from the Latin words rectefacere, meaning to improve. Modern distillation derives its ability to produce almost pure products from the use of multi-stage contacting. In distillation column disturbances comes from many side because the interaction occurring the feed and the product are difficult to identify. The disturbance comes from either side i.e. the feed flow rate, feed composition, inside the column pressure, from the cooling water etc. From these disturbances number of challenge in running plant in control problem and so we can do lot of research in different discipline like electrical, mechanical and chemical.

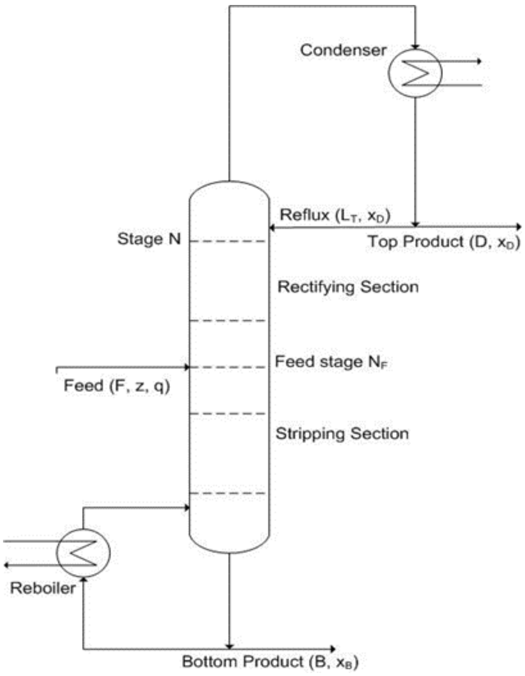

Figure 1. A Two-product Distillation Column

To study the behaviour of distillation column first we should make the model for distillation column. We can easily understand behaviour of column by modelling , can guess next reaction and therefore devise a control structure for the column. In the present work study some important techniques in distillation column modeling. These MESH equations have been solved by making use of the solver 'fsolve' in MATLAB, which can solve various non-linear equations simultaneously. The model has been simulated under different simulating conditions, viz., different feed conditions (saturated vapour, half vaporized and (saturated liquid) and different feed compositions. A MATLAB code has been developed in order to simulate the model for different simulating conditions in order to study the impact of the different parameters on the steady-state performance. A brief outline of the work presented in we made the model of continuous distillations in part II, the modeling of our distillation column is detailed in part III, the simulation results are shown in part IV, and the conclusion and future work are presented in part V of this paper. Objective of the presented work to develop the code in MATLAB for distillation column, to validate the code with available data, to study affect the operating variable.

II. MODELING OF CONTINUOUS DISTILLATION COLUMNS

We can distinguish the modeling of distillation column in three group: fundamental modeling, empirical modeling and hybrid modeling [1]. In fundamental modeling, we made the model on conservation of physical properties such as mass, energy and momentum and ii depend on the accuracy of assumption we use simple to rigorous model.

Simulation calculations for the distillation column have been made in order to study its behaviour when feed of different types are fed, for example, saturated liquid, saturated vapor and half vaporized, with the design and operation of the column remaining unchanged. By running the simulations for the distillation, it has been actually tried to establish the thermal condition of the feed that leads to a greater methanol concentration in the liquid phase inside the column. The simulation calculations indicate that the latter is obtained by means of feeding a saturated liquid feed. It is also economical to feed the saturated liquid feed to the column, which is beneficial from two viewpoints, i.e., from the viewpoint of separation as can be seen from the graphs and also from the heat economy viewpoint. To make the model from this method advantage is global validity, accuracy. This method of modeling has the advantage of global validity, accuracy. However, this method is quite complex for controller design with huge amount of computation and simplifications are often needed [1].

In the empirical modeling uses the data from the running of the column to build the relationship between the input and the output. With this method we do not need to understand the inner dynamics of the column, and the computation can be reduced. But in using this method we have to carry out experiments on the real column, and the results may not be applied for other column, even the results from one column can be different if the column's conditions are different between the experiment and the actual operation of the column.

In the hybrid modeling, as we know the word hybrid, it is combines the fundamental modeling and the empirical modeling. As it is hybrid modeling, it has advantages of the other two, but for that we need well structural model for that which part of model model to use fundamental technique and which part to use empirical data. We made our model with fundamental modeling, but empirical model is dominantly use in industries. It is used because of that it is easy to understand the dynamics The reasons that we want to understand the dynamics of the distillation columns, and since the empirical model may not be used to predict the behaviour of the system at other operating conditions" [4].

Martin-Sanchez (1976) developed the adaptive predictive control system which is related to the traditional dead-beat control idea of bringing a system to its final state or set point in minimum time. It is characterized by the following principles:

(1) At each step a future desired process output is generated, and the control input is computed in order to make the predicted process output equal to the desired process output.

(2) The predicted output is based on an adaptive predictive (AP) model, whose parameters are estimated by a recursive estimation law the objective of minimizing the prediction error.

(3) The previously mentioned desired process output belongs to a desired output trajectory, that satisfies a certain performance criterion, e.g., this trajectory can start from the current 'state' of the plant and evolve according to some chosen dynamics to the final desired set point.

Cott et al. (1986) presented selection techniques for approximate models of process model based controllers for distillation columns. In their article they state what the qualities of an ideal model ought to be and then go on to develop a selection procedure using the following guidelines:

(1) Model Accuracy

(2) Model Selection Procedure

(3) Model Parameter Update.

Luyben et al. extensively covers the dynamics of multicomponent distillation columns, and presents an algorithm using Euler's method to solve the differential equations. In his approach almost all possible nonlinearities are eliminated by local linearization, using the following

Assumptions:

(1) There is one feed plate onto which vapour and liquid feed are introduced.

(2) Pressure is constant on each tray but varies linearly up the column.

(3) Coolant and steam dynamics are negligible in condenser and reboiler.

(4) Vapor and liquid products are taken off the reflux drum and in equilibrium. Dynamics of vapor space in reflux drum are negligible.

(5) Liquid hydraulics are calculated from the Francis weir formula.

(6) Volumetric holdups in the reflux drum and column base are held constant by changing the bottoms and distillate rates.

(7) Dynamic changes in internal energy on trays are negligible compared with latent-heat effects, so the energy equation on each tray is just algebraic. Luyben also presents a code for the algorithm in his text. However, with the availability of some differential equation solving packages, Euler's method is inefficient by contrast.

Sourisseau and Doherty (1982) studied various different dynamic models and classified them according to the state variables employed. Following their definitions, a model in which the state vector consists of only liquid compositions was called the C-model. If both compositions and enthalpies are included, the CE-model results. The most complex model is the CHE-model and has a differential equation for each state variable on each tray (composition, holdup and enthalpy). The constant molar-overflow model (CMO-model), assumes fast holdup and energy changes as well as fixed liquid and vapor rates at all times.

S. Skogestad did a critical survey of literature on dynamics and control of distillation columns up until 1991. The paper summarized the simplifications of the rigorous model since no references had been found on solving all the equations of the rigorous model. The simplifications are aimed to the vapor dynamics, to the energy balance and to the liquid flow dynamics. The paper recommends not neglecting liquid dynamics (i.e. not assuming constant liquid holdups) due to the fact that the initial response, an important factor in feedback control, is largely affected by the liquid holdups.

B. Wittgens and S. Skogestad carried out an evaluation of dynamic models of distillation columns with emphasis on the initial response. They found out that the most important parameters are the liquid holdup, the liquid hydraulic time constant and the vapor constant that represent the initial effect of a change in vapor flow on liquid flow.

Abdulla et al. have done a quite complete review on the recent nonlinear modeling applications in continuous distillation column. The summary states that the empirical modeling has been preferred in industry because of its simplicity compared to the fundamental model; and the current development focuses on hybrid models, which can exploit the advantages of both fundamental model and empirical model; and that the neural network method is used the most to combine with the fundamental model in empirical modeling.

In the case of fundamental modeling, the model is often simulated to understand the column's dynamic behaviour. The development of distillation column's simulation has been going along with the growth of computing capacity. As of 1930s and 1940s only graphical methods and

Simple short-cut models were used to get insights of the steady-state behaviour of the distillation columns. The fast-growing of computing power has allowed the use of more complex and rigorous models. Computer programming and the numerical methods to solve the differential equations play an important role.

A MATLAB code has been developed in order to simulate the model for different simulating conditions in order to study the impact of the different parameters on the steady-state performance

III. MODELING OF THE APC

The APC (Advanced Process Control) column is a pilot distillation column that has 15 trays and equipped with a DCS control system. The feed is positioned at tray 7. In the model the following assumptions are made:

1. Binary mixture, the feed contains only two components
2. The pressure inside the column is fixed by controlling the cooling water
3. Constant relative volatility, $\alpha = 1.5$
4. Constant molar flows
5. No vapor holdup, the vapor holdup on each tray is negligible
6. Linear liquid dynamics
7. Equilibrium on all stages
8. Total condenser, there is no vapor holdup in the condenser

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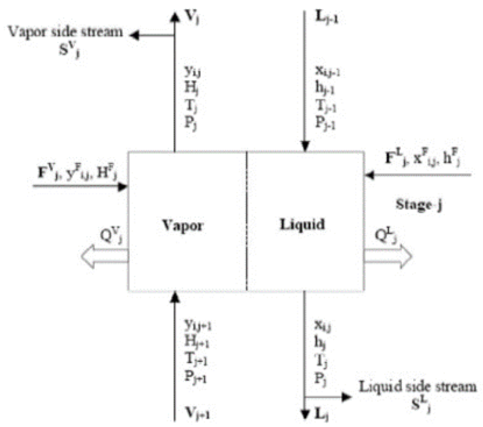
STEADY-STATE MODELING OF A DISTILLATION COLUMN

A rigorous steady-state column model was developed using MESH equations which actually represent the behaviour of the column where x_i and y_i is the composition of the light component and heavy component on tray i respectively. At the feed stage (N_F=7). We have Figure shows the schematic of a separation stage. The model consists of mass balance, equilibrium relation, summation equations and energy balance, which are collectively known as MESH equations



Mass Balance

The model equations for a general 'j^th' stage and 'i^th' component are represented as:

$$L_{j-1}\, x_{j-1,I} + V_{j+1} y_{j+1i} + FZ_{j,i} - (V_j + s_j^v)\, y_{j,I} - (L_j + s_j^l) = 0 \qquad \text{.............1}$$

And in terms of the flow rate of components, above equation can be written as:

$$l_{j-1,I} + V_{j+1,i}\, ,f_{ji} - v_{j,i} - s_j^l - lj,i - s_{ji}^v \quad = 0 \qquad \text{...............2}$$

where

$$l_{i,j} = L_j\, x_{ij} \qquad \text{...............3}$$

$$V_{i,j} = V_j y_{ij} \qquad \text{................4}$$

$$V_j = \sum_{i=1}^{c} Vi,j \qquad \text{.................5}$$

Equilibrium Relationship

The compositions of the streams leaving a stage are in equilibrium. Therefore, the mole fractions of the com ponent 'i' in the liquid and vapor streams leaving stage 'j' are related by the equilibrium relation shown in the equation given below:

$$y_{j,i} = K_{j,i}\, x_{j,I} \qquad \text{....................6}$$

Energy Balance

The total energy balance for 'jth' stage is given by:

$$L_{j-1}\, h_{Lj-1} + V_{j+1}\, h_{vj+1} + F_j h_{F,j} - (L_j + V_j)\, h_{Lj} - (V_j + W_j)\, h_{vj} - Q_j = 0 \qquad \text{.....................7}$$

The composition of the heavy component is related to the composition of the light component via the relative volatility formula

$$y_i = \frac{\alpha x_i}{1+(\alpha-1)x_i} \qquad \text{..............8}$$

The liquid flow dynamics is considered due to its important effect on the initial response of the column. The formulas for the liquid holdup are:

$$L_i = L_{0,b} + \frac{Mi - Mo,i}{\tau} + (V_{i-1} - V_0)\ \alpha \qquad \text{..................9}$$

$$L_i = L_{0,b} + \frac{Mi - M0,i}{\tau} + (V_{i-1} - V_0)\ \alpha \qquad \text{....................10}$$

for i from N_F+1 to N_T-1 where L0 is the nominal reflux flow and M0i is the nominal reboiler holdup (kmol) on stage i. These values are achieved after we do steady state simulation (see Table 1). τ is the time constant for liquid dynamics, in this model it is chosen to be 0.063 (min), and λ represents the effect of vapor flow on liquid flow. In the simulation we ignore this effect by setting λ=0.

$$L_{0b} = L_0 + q_{F0} F_0 \qquad \text{....................(11)}$$

in which F_0 = 1(kmol/min) is the nominal feed rate, q_{F0} = 1 is the nominal fraction of liquid in the feed.

IV. SIMULATION RESULTS AND DISCUSSION

The main objective is to modelling and simulation is to check the response of distillation column. In the present work we want to see how the column respond when the change due to disturbance in feed and output composition. We found that the our main focus is to control the distillation column because it effect the dynamic of column. We do the simulation with the help of MATLAB. We run the program till the steady state. The steady state data is shown in figure.

TABLE I. STEADY STATE DATA OF THE COLUMN

Z_F	A	N	N_F	X_D	X_w	D	B
0.5	2.10	9	4	0.92	0.07	0.5	0.5

After simulating, when we get the steady state, we check the composition under different disturbance. We choose a step change in feed flow rate because of most frequent disturbance. We check the response in the composition of the light component at the reboiler (X_B) and at the condenser (X_D) when the magnitude of the step change. We must the level distillate and bottom tank kept constant simulating by changing the distillate and bottom (B) flows. In our model both level control by PI control with gain equal to 8.

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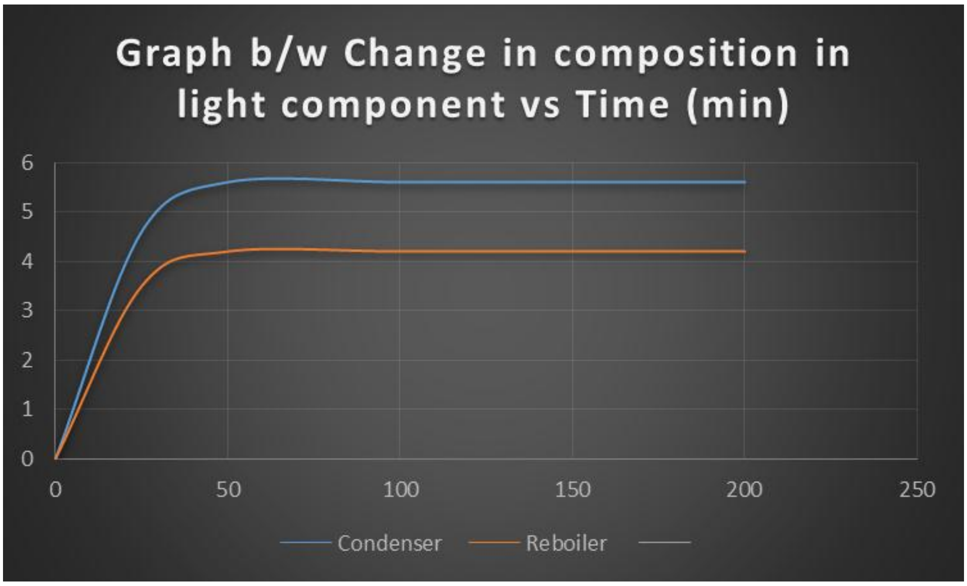

Fig. 2 shows the changes in compositions due to 1% increases in feed flow rate.

Figure 2. Composition responses to 1% step increase in feed flow rate For 1% increase in feed flow rate, the response of X_D has a time constant of about 17 minutes while the response of X_B has a time constant of 11 minutes. The output result showing in the curve is the response of a first order system in varying the time constants as we know the (the value of reaches 63.2 percent of its ultimate value when the time elapsed is equal to one time constant), which is good deal with the other author.[7],[8].

In digram 3 , after the simulating when we increase the feed flow rate 10% which are 15 minutes and 10 minutes respectively. We can see the responses in this case are faster than in the case of 1% increase in feed flow rate. We simulate our model with two step change 1% to 20% . The output result shown in table II.

Table II . Time constants (in minutes) of the composition changes due to different feed flow rate perturbations

	1%	10%	15%	20%
X_D	22	20	16	15
X_W	16	17	13	10

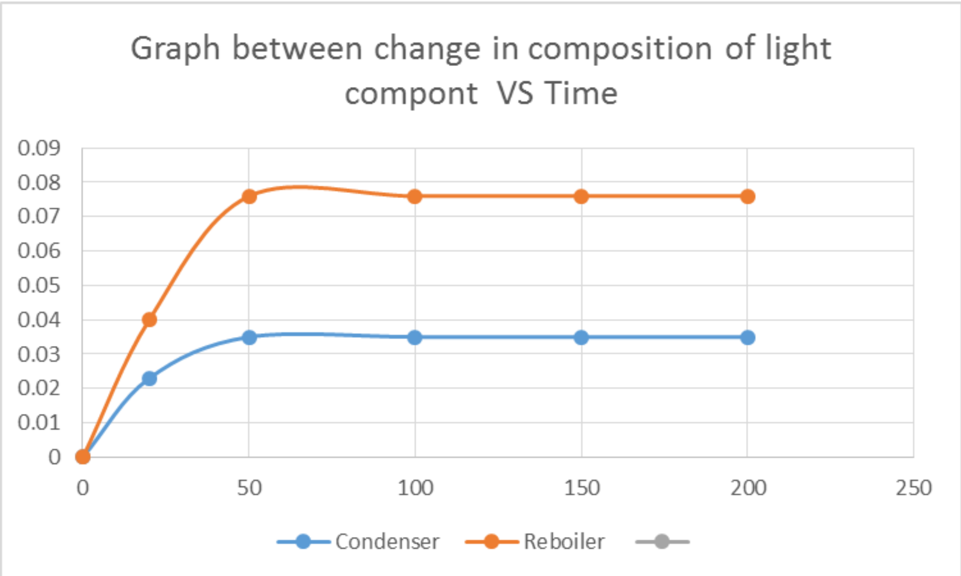

Figure 3. Composition responses to 10% step increase in feed flow rate

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After the simulating from the simulation results it is easily observed that the slow respond of the composition of the distillation columns which has been in good agreement with other author[8].

$$\tau_{sc} = \frac{M_I}{I_{sln\, s}}$$

$M_I = \sum_{i=2}^{N} M_i$ is the total holdup of liquid inside the column

$I_s = Dx_D\ (1- X_D) + BX_B\ (1-X_B)$ is the "impurity sum"

And $S = \frac{XD(1-XB)}{(1-XD)XB}$, is the separation factor.

Substituting the steady state values from Table 1 to (13) above we get τ = 18 (minutes).

When we increase in the feed flow rate 1% to 10%, we found that the time constant is consistent, but also we found that it is not consistent when we increase it to 10% to 20%. We can conclude it to it is good agreement with the Skogestad and Morari.

Further we check the response in disturbance in the feed composition .We increase input in the light component to the feed in step input 1%,5%, 10%, 20%.There should be change composition responses in this case also resemble a first-order response. The response to 5% step increase in feed composition is plotted in Fig. 4.

In next table we can see the time constant of the responses.

Table III. Time constants (in minutes) of the composition changes due to different feed composition perturbations

	1%	10%	15%	20%
X_D	18	16	16	11
X_W	19	17	19	19

From the result we can easily understand when we change the magnitude of the disturbance, the time constants don't vary much. It is obviously seen from the comparing the steady state gain, the response due to change in the feed composition is always greater than the response due to change in feed flow rate. We also check the dynamics of the column is the effect of internal and external flows on the compositions of the products. We simulate a change in external flow by increasing the reflux rate L while keeping the boilup rate V constant. The composition response to 0.1% increases in L and V is shown in Fig. 5.

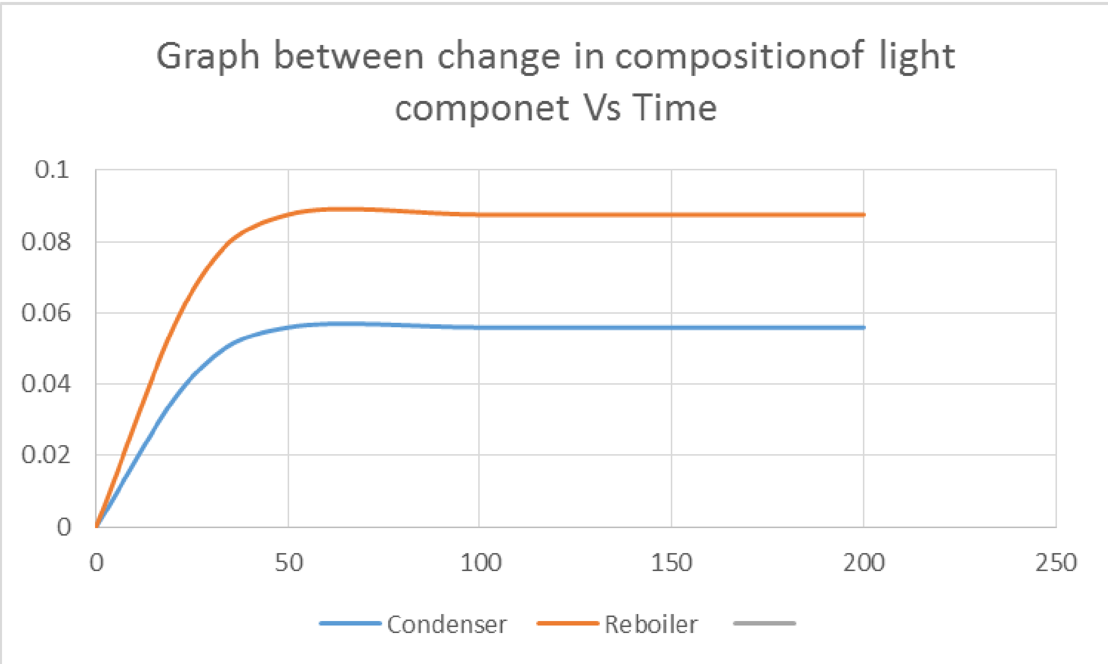

Figure 4. Composition response to 1% increase in feed composition

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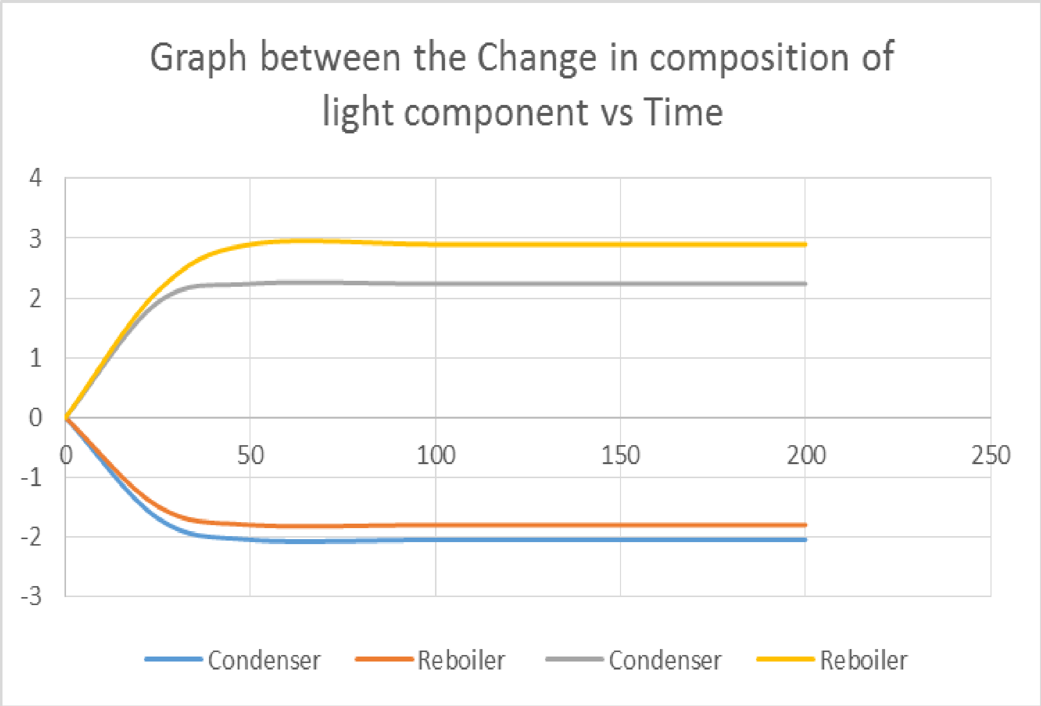

Figure 5. Composition changes due to 0.1% increases in L and V

In the case of increasing L with V being constant we can see the changes in liquid compositions of the light component in the reboiler (X_B) and in the condenser (X_D) are both positive. This means the light component gets purer in the distillate tank and the heavy component gets more impure in the bottom tank. In the opposite case, when we increase V and keep L constant we get the opposite result: the heavy component gets purer in the bottom tank and the light component gets more impure in the distillate tank. In both cases the time constants are close to 14 minutes.

An internal flow was simulated by applying a simultaneous increase in L and V, while keeping the product rates, D and B, constant. Fig. 6 shows the composition response to 10% increase in both L and V.

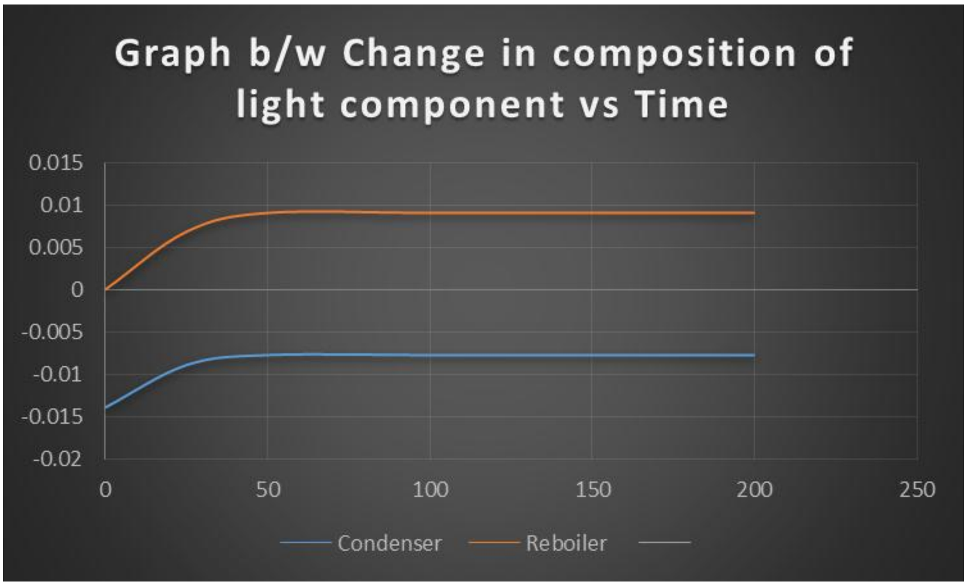

Figure 6. Composition changes due to 10% increase in both L and V

From the simulating result, it is shown that bottom fraction is negative while distillate fraction is positive, from that we can say that both product is this purer form. Also from the result we can alter between internal and external flow. When we do small change in external flow (1%) will make the products compositions change with different directions while a much bigger change in internal flow (20%) will make the products compositions change with the same direction. This is in better agreement with the results obtained by model presented by author.

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V. CONCLUSION AND FUTURE WORK

In this present work we made a model of a continuous binary distillation based on mass balance and constant relative volatility. With the help of MATLAB we simulate our model. The simulation results show that the composition responses are close to the response of a first order system. We can formulate response if the change is small for the given feed flow rate can be formulated if the change is small. We also check that the we get larger gain response due the response due to change in feed flow rate. Our work can be extended with the help of program, we can simulates for more the responses of the compositions to other disturbances. We can validate our model with running plant. In the present we consider one variable and in future we do it for multi variable system.

Nomenclature

B	Bottom product flow rate (kmol/min)
D	Distillate product flow rate (kmol/min)
F	feed flow rate (kmol/min)
IS	Impurity sum
L	liquid flow rate (kmol/min)
M	liquid holdup (kmol)
MI	total liquid holdup inside the column (kmol)
N	number of physical trays (N=15)
NF	tray number at feed position (NF=7)
NT	Number of theoretical trays, including the condenser
S	Separation factor
V	Vapor flow rate (kmol/min)
y	Liquid composition of the light component
x	Vapor composition of the light component

Greek letter

α	relative volatility
λ	parameter for the effect of vapor flow to liquid flow
τ	time constant for liquid flow dynamics
μ	molar chemical potential (jmol-1)
σ	surface tension (N m^{-1})

Subscripts

B	Bottom tank
D	Distillate tank
i	tray number
S	sum
sc	short cut

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